



# Strategies For The Use Of Ensemble Information in Data Assimilation

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Adjoint Workshop, 13 October 2011



# Outline

- Motivation.
- The Issues.
- Where Next?



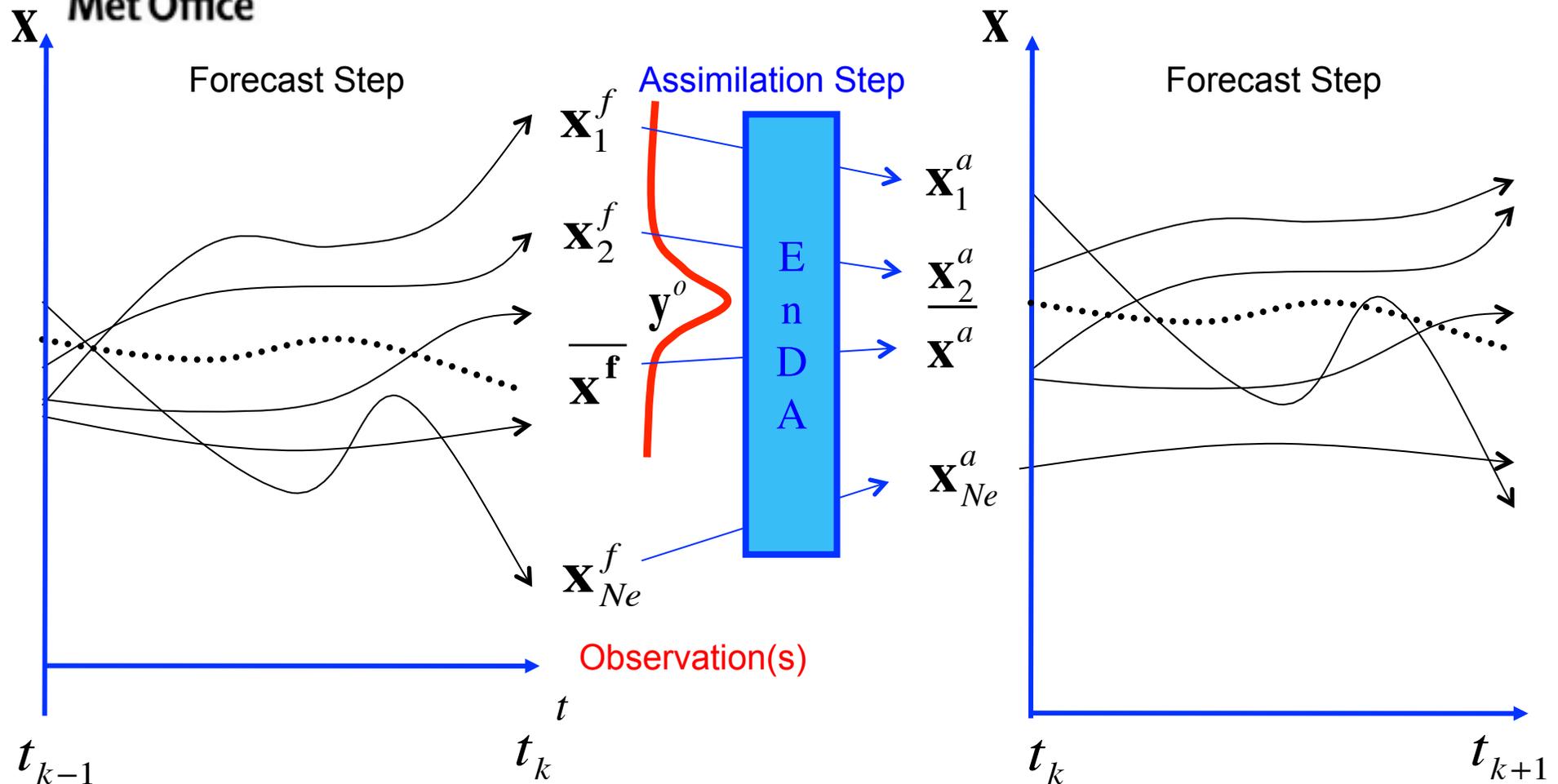
# Motivation

- Current atmospheric DA conceived in 80's-90's. Time for a review!
- Comparison of EnDA vs VarDA indicates competitive performance.
- Computational efficiency of 4D-Var on next-gen HPC under question.
- Forecast model likely to change radically in next 5-10yrs. Should DA?
- Increasing range of applications for DA. Should effort be more 'seamless'?
- What is best method for Met Office for next 5-10 years?



Met Office

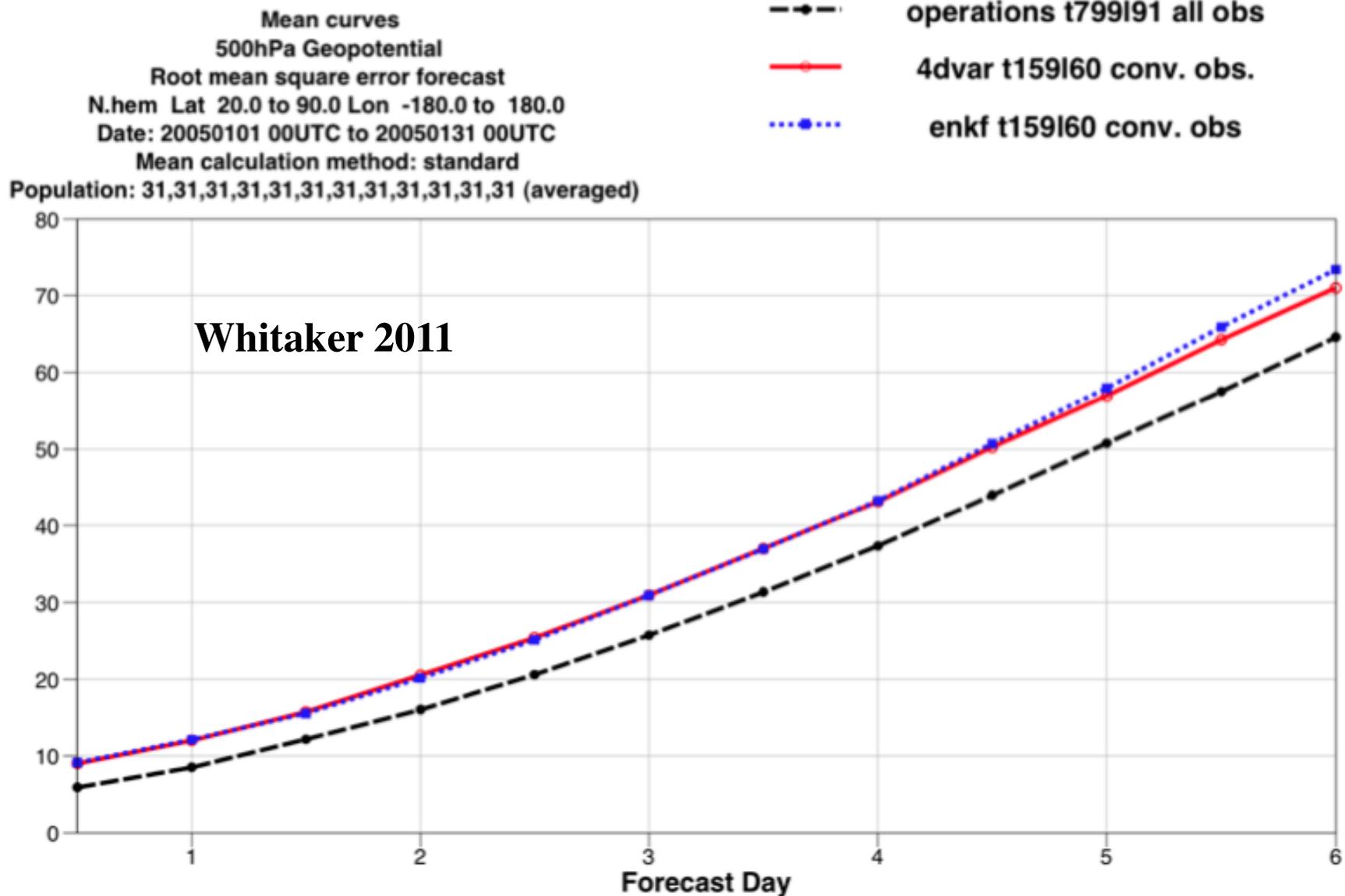
# Ensemble Data Assimilation (EnDA)



- Majority of EnDA cost is in forecast step (compare with 4D-Var).
- Parallelism easier to achieve with EnDA (at least in expensive forecast step).

# EnKF - Current state of the art

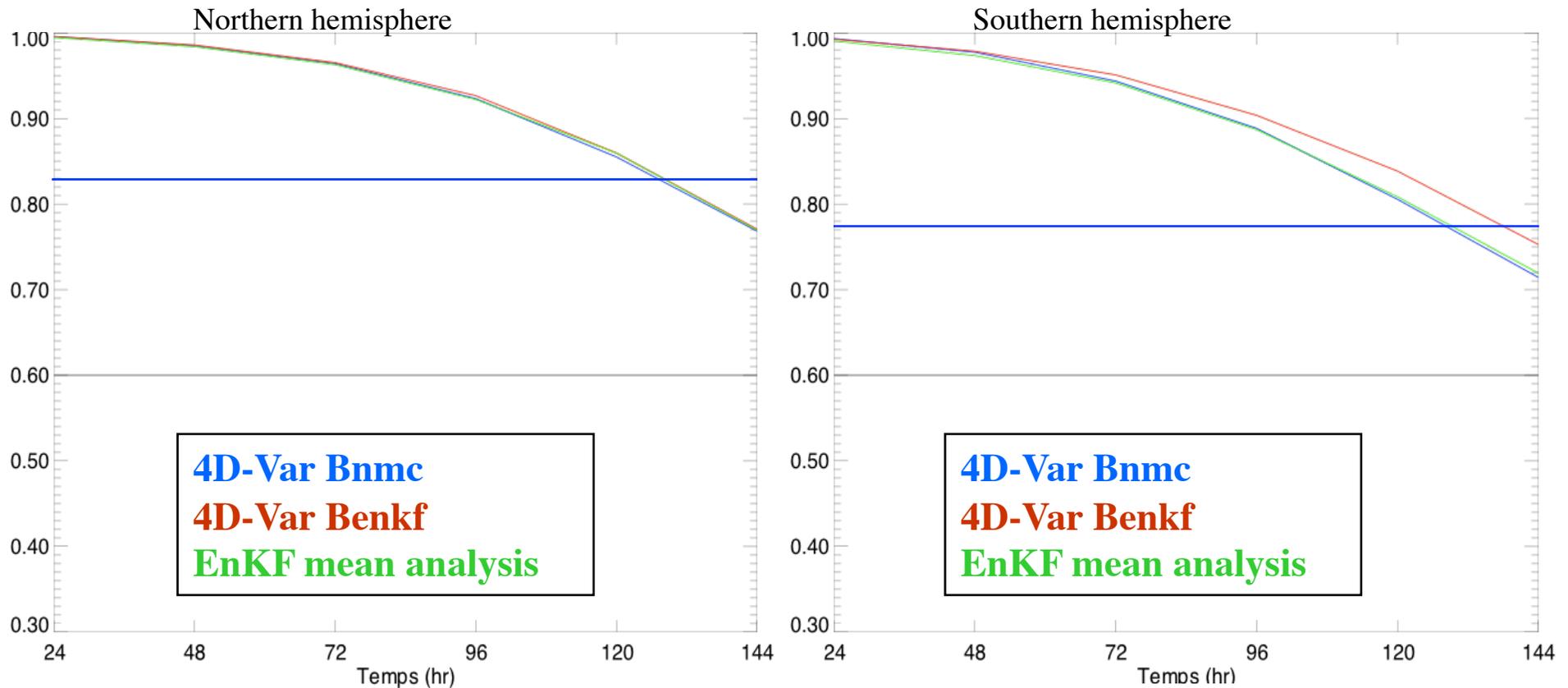
*ECMWF EnKF vs 12-h 4DVar (T159), conv obs only*





# Comparison of 4D-Var/EnKF (Mark Buehner, EC)

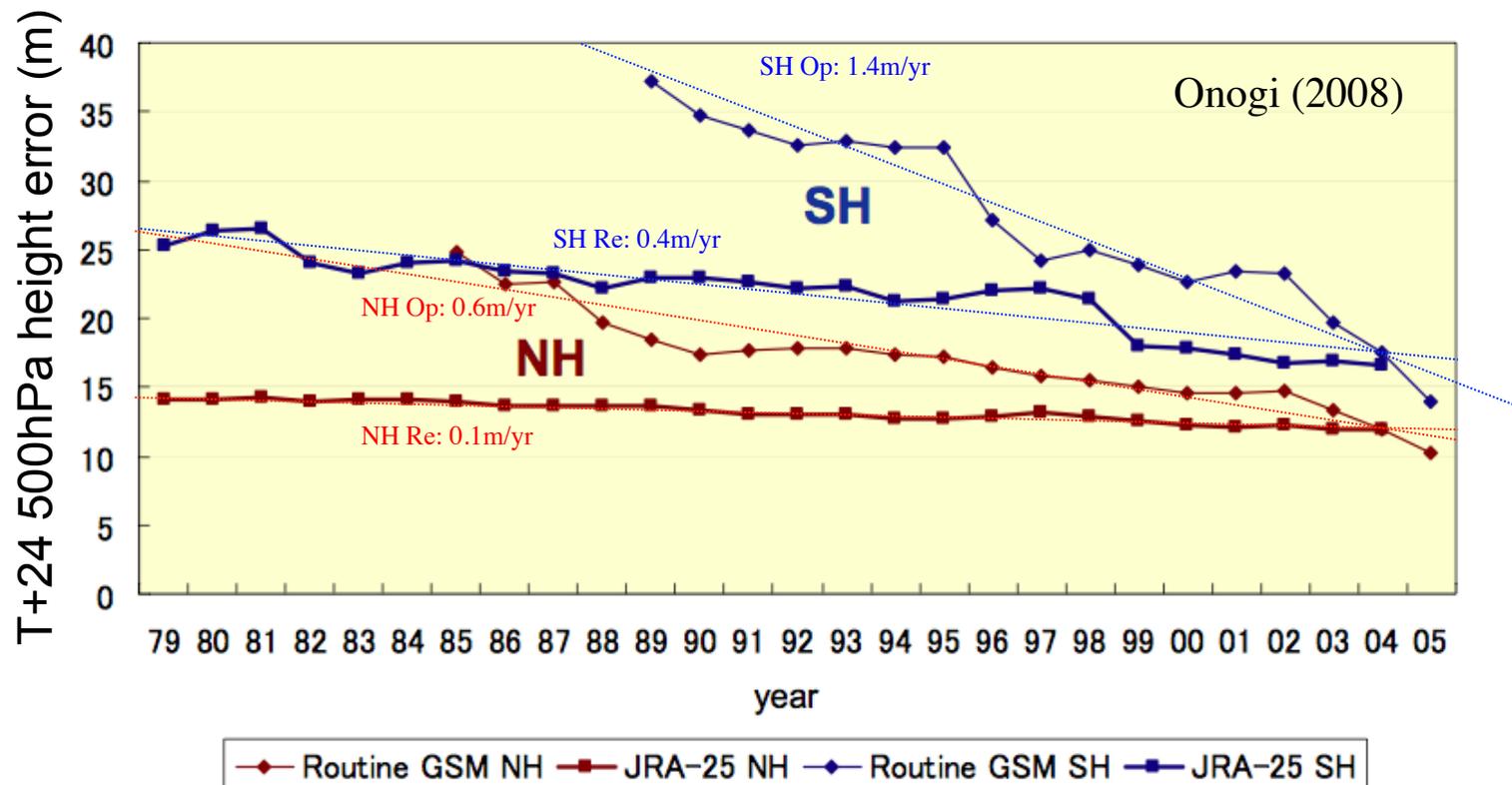
\*\*\*Verifying analyses from 4D-Var with Bnmc\*\*\*



- EnKF/4D-Var similar performance
- Combined 4D-Var + EnKF covariances even better, but a luxury?



# Relative Contribution of Changes In NWP+DA vs. Observing Network (JMA Reanalysis/NWP Performance)



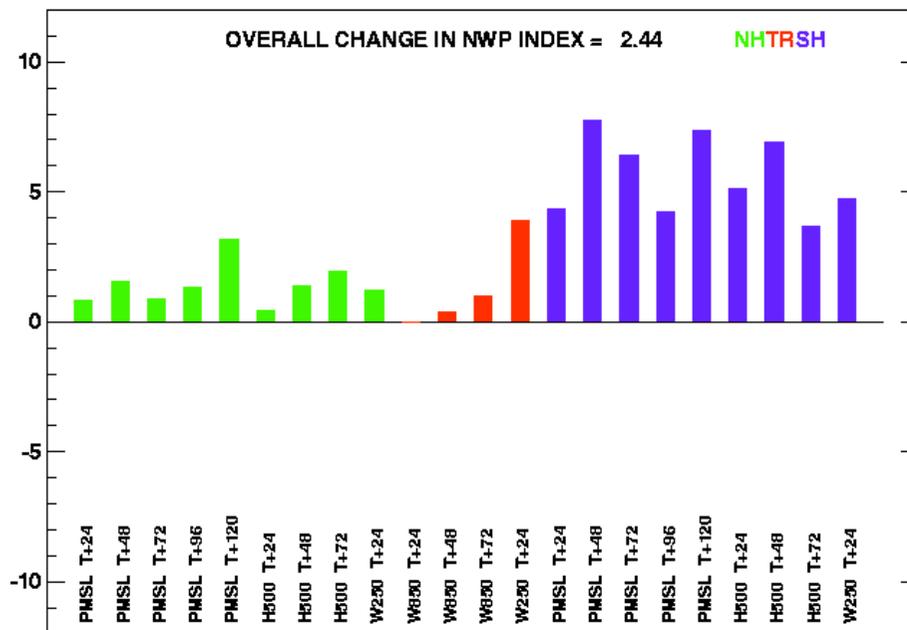
- Most of forecast benefit over 25yr period due to better models and DA systems, rather than observations (especially in NH).
- Caveat: Not true for all metrics (e.g. precipitation shows bigger impact of obs).



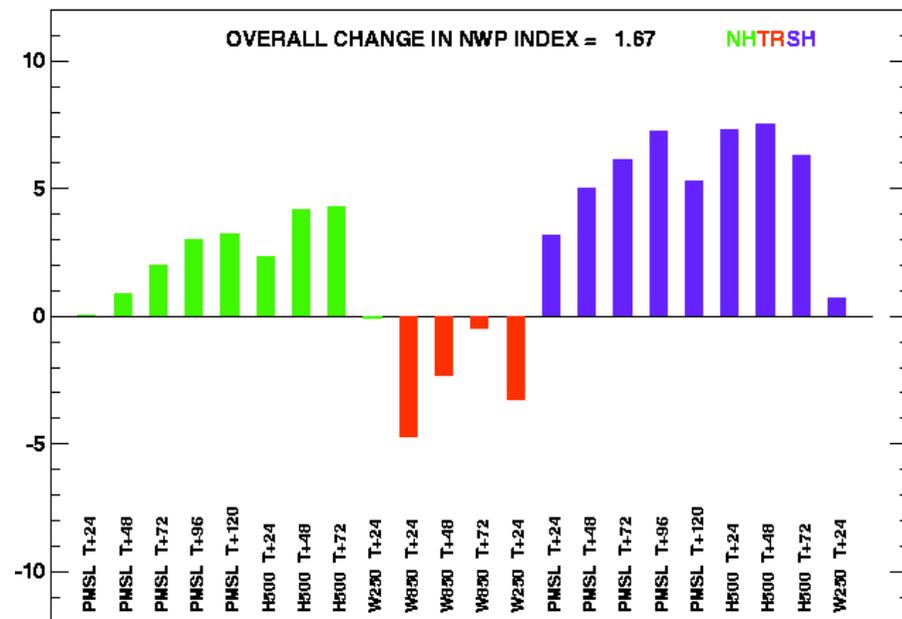
# July 2011 Global DA/SA Upgrade

%Reduction in RMSE For Critical Met Office Forecast Parameters:

**Vs. Observations**



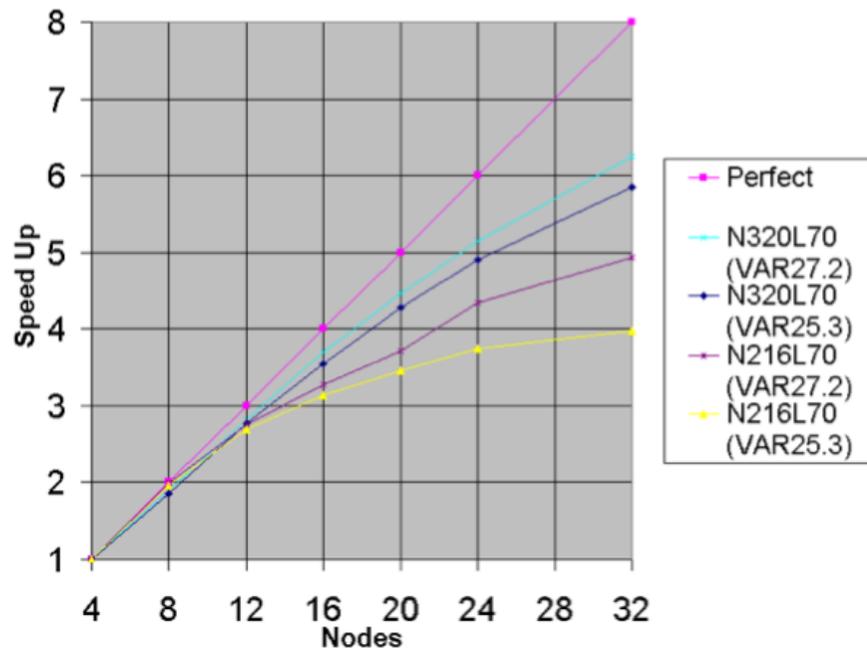
**Vs. Met Office analyses**



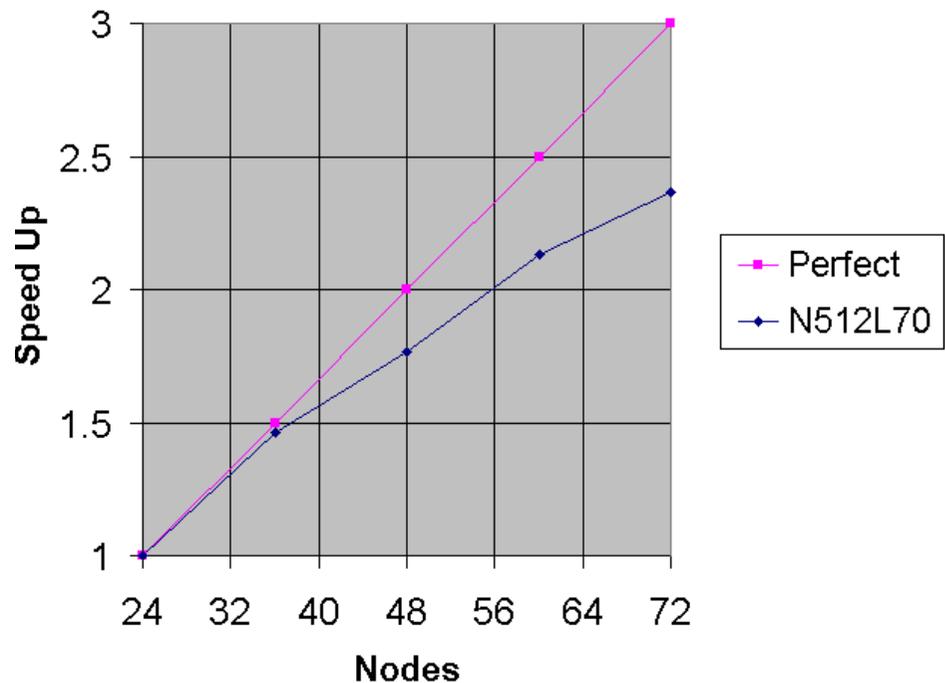
- Biggest reduction in overall global forecast error for many years.
- First time in memory that all parameters have reduced error vs obs. (usually a mix).



# Computational Efficiency: 4D-Var Scalability on IBM P6



N216/320 (60/40km) 4D-Var

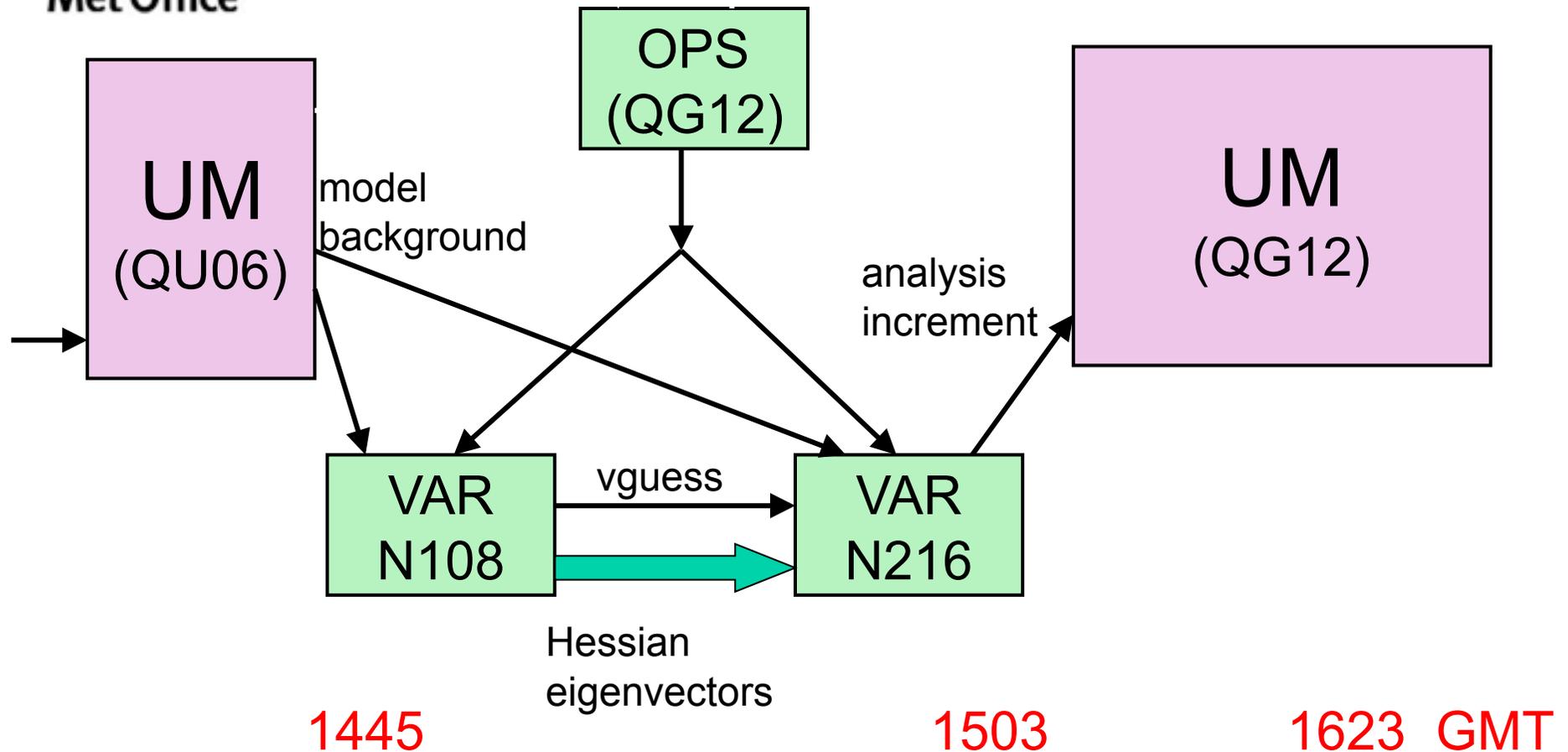


N512 (25km) 4D-Var

- Code optimization + increased resolution improve scalability.
- Significant algorithmic changes unavoidable for next-generation DA, e.g. weak-constraint 4D-Var, reduced cost linear model, etc.



## Towards 'Quasi-Continuous' 4D-Var



- Preconditioning reduces cost of final N216 4D-Var from 21mins to 13mins.
- Shifts some of cost of 4D-Var to before critical obs. cut-off time, BUT
- Increased complexity + total cost.



# 4D-Var

- The cost function  $J$  is typically

$$J[\mathbf{x}(t_0)] = \frac{1}{2} [\mathbf{x}(t_0) - \mathbf{x}^b(t_0)]^T \mathbf{B}_o^{-1} [\mathbf{x}(t_0) - \mathbf{x}^b(t_0)] + \frac{1}{2} \sum_{k=0}^K [\mathbf{y}_k - \mathbf{y}_k^o]^T \mathbf{R}_k^{-1} [\mathbf{y}_k - \mathbf{y}_k^o]$$

$$(\mathbf{y}_k = HM_k [\mathbf{x}^b(t_0) + \delta\mathbf{x}(t_0)] = HM_k [\mathbf{x}^b(t_0)] + \mathbf{H}\mathbf{M}_k \delta\mathbf{x}(t_0))$$

- $M$  is nonlinear model.  $\mathbf{M}$  is linear model (not usually tangent linear).  $\mathbf{B}_o$  is the background error covariance (includes variable transformation e.g. streamfunction, potential vorticity, etc).
- Efficient minimization of cost function requires gradient

$$\left[ \frac{\partial J}{\partial \mathbf{x}(t_0)} \right]^T = \mathbf{B}_o^{-1} [\mathbf{x}(t_0) - \mathbf{x}^b(t_0)] + \sum_{k=0}^K [\mathbf{M}(t_{k+1}, t_0) \mathbf{H}_k^T \mathbf{R}_k^{-1} (\mathbf{y}_k - \mathbf{y}_k^o)]$$

- $\mathbf{M}^T$  is the transpose (adjoint) of  $\mathbf{M}$ .  $\mathbf{M}(t_k, t_0)^T = \prod_{j=0}^{k-1} \mathbf{M}(t_{j+1}, t_j)^T$



# The Ensemble Kalman Filter (Example: Stochastic EnKF)

- Forecast step (for ensemble member  $n$ , observation time  $i$ ):

$$\mathbf{x}_n^f(t_i) = M_{i-1} [\mathbf{x}_n^a(t_{i-1})]$$

$$\mathbf{P}_{ens}^f = \frac{1}{N_e - 1} \mathbf{X}^f \mathbf{X}^{fT}$$

- Update step:

$$\mathbf{x}_n^a(t_i) = \mathbf{x}_n^f(t_i) + \mathbf{K}_{ensi} (\mathbf{y}_i^{op} - H_i(\mathbf{x}_n^f(t_i))),$$

$$\mathbf{K}_{ensi} = \mathbf{P}_{ens}^f(t_i) \mathbf{H}_i^T (\mathbf{H}_i \mathbf{P}_{ens}^f(t_i) \mathbf{H}_i^T + \mathbf{R}_i)^{-1}$$

- $\mathbf{y}_i^{op}$  are observations perturbed with random noise (called **stochastic** EnKF).

- No linear model so EnKF less tied than 4D-Var to particular model.
- Adjoint not required.
- Covariance modelling still required (localization, inflation, etc).



# Plans For NWP Model: Spring 2013 (Tentative)

## Global

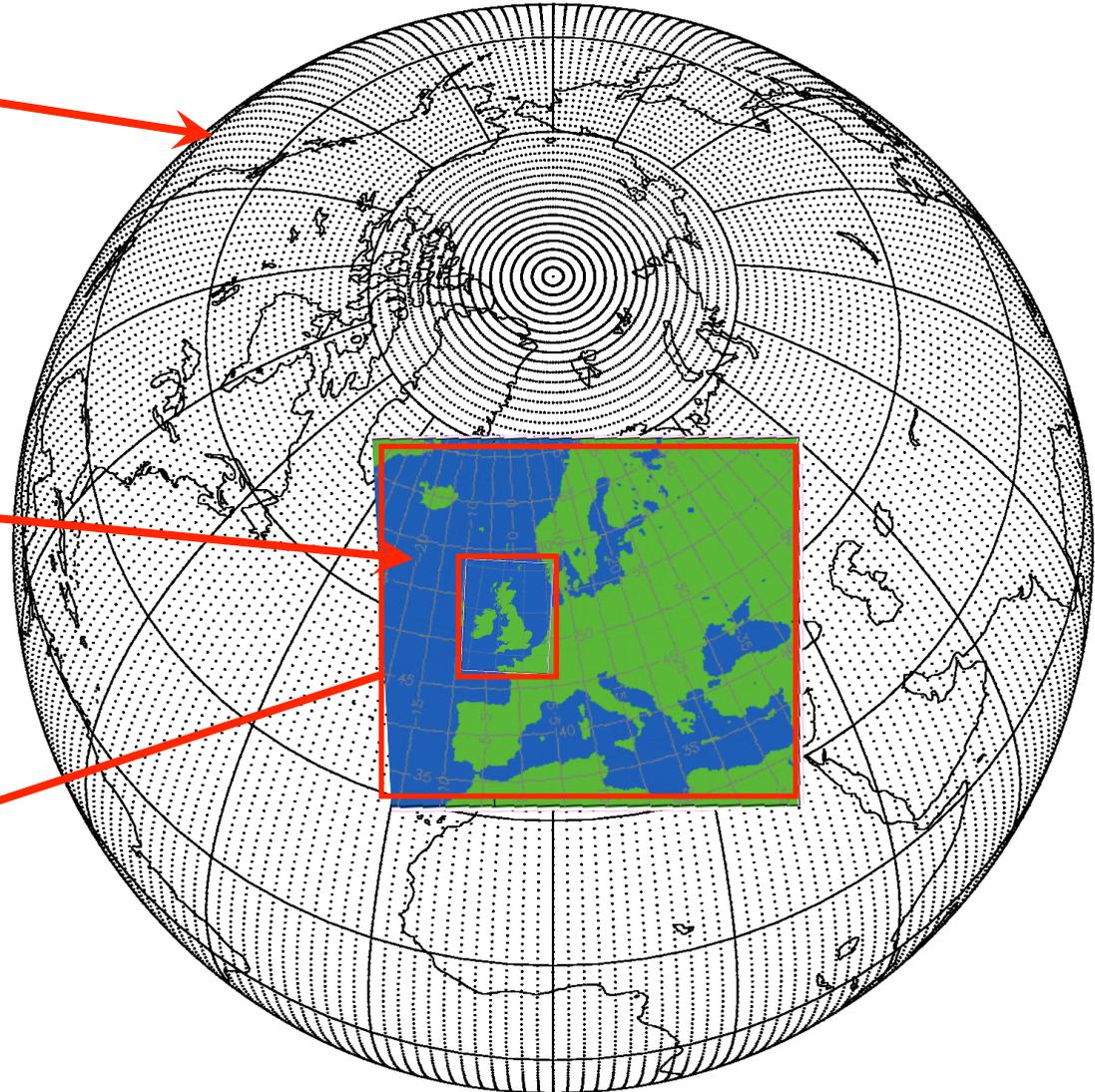
- 16-20km 85L (85km top)
- Hybrid 4DVAR (40km inner-loop)
- 60 hour forecast twice/day
- 144 hour forecast twice/day
- 48/12member 40km MOGREPS-G 4\*

## MOGREPS-EU

- Common NWP/reanalysis domain.
- 12Km 70L (40km top)
- 3D-Var (or NoDA)
- 48 hour forecast
- 12 members ; 4 times per day

## UKV

- 1.5km 70L (40km top)
- 3DVAR (hourly)
- 36 hour forecast, 4 times per day
- 12 member 2.2km MOGREPS-UK

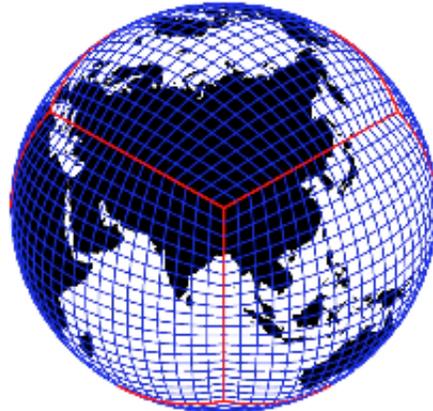




# Operational NWP Models: 2020 (Exceedingly tentative!)



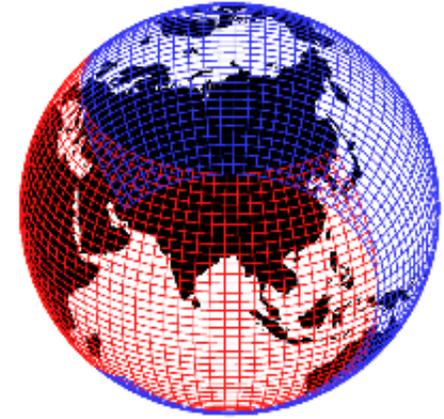
**Lat-lon**



**Cubed-sphere**



**Icosahedral**



**Yin-Yang**

- Dynamical core development:
  - 2012 – ENDGAME (ND with  $v$  at poles, higher order accuracy)
  - 2015 – Ying-Yang option (stitch two ND regional domains together).
  - 2020 – Next-Generation MetOffice Dynamical Core (GUNGHO)

- Radical change to dynamical core – need to rewrite 4D-Var?
- Or, move to less model-dependent DA?

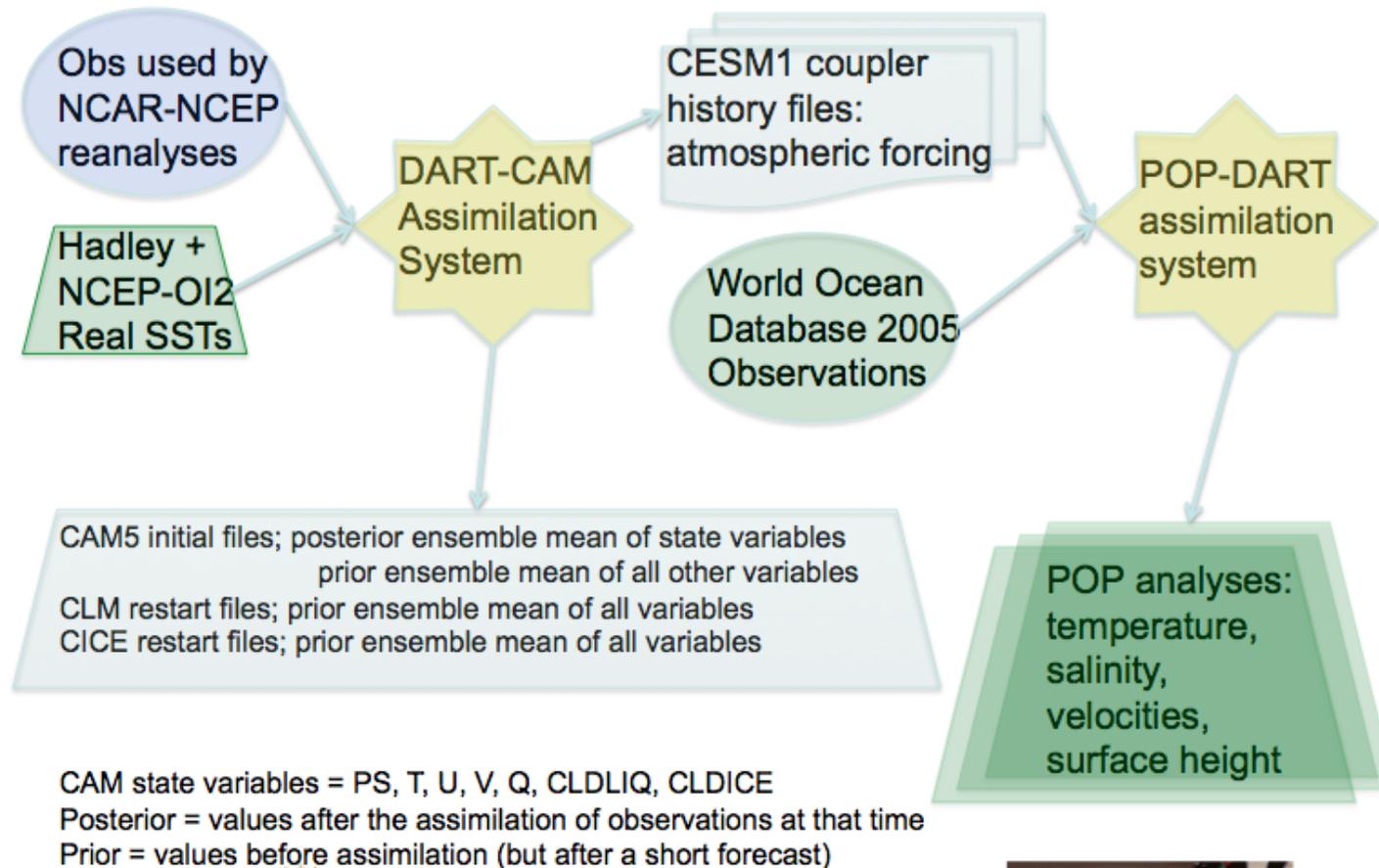


# DA For the Earth System Model

- MetO DA activities:
  - Atmosphere: VAR (Hybrid three/four-dimensional variational DA)
  - Ocean: NEMOVAR
  - Land: Nudging (now) -> EKF (2012) -> EnKF (later).
  - Coupled DA: (WG formed, begin with coupled initialization).
  - Not yet: Space weather, Chemical, Sea-ice.

- Increasingly diverse applications of DA.
- Do we need to rationalize range of techniques/systems or rely on increased application-specific collaboration (e.g. NEMOVAR)?
- Do we need strongly-coupled ESM DA (atmosphere-ocean-land-etc). If so, how does that influence the design of next-generation DA algorithms?

# POP-DART (NCAR – Raeder et al)



- Weakly-Coupled Data Assimilation (separate DA, couple analyses).
- Need for strongly-coupling (unified DA) not yet clear.



Met Office

## Where Next?

EnDA is the future, but which approach?



# Where we are now: Hybrid Variational/Ensemble DA

## Scientific Motivation:

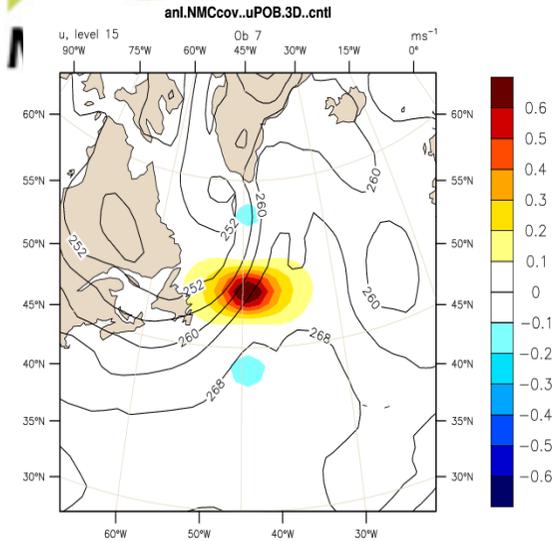
- 4D-Var provides flow-dependent covariances via the linear (perturbation forecast) model. However, still limited by climatological background error covariance.
- Current MetO Ensemble has only 24 members - likely to suffer from significant sampling error for DA.
- Mix (hybrid) covariances can ameliorate weaknesses of both VarDA and EnDA.
- Lorenc 2003 indicates hybrid equivalent to deterministic EnSRF - so no real incentive to consider replacing with EnSRF.

- Hybrid permits leveraging of additional attractive features of variational algorithm: outer-loop for nonlinear DA, simultaneous treatment of all observations, balance constraints, etc, etc.

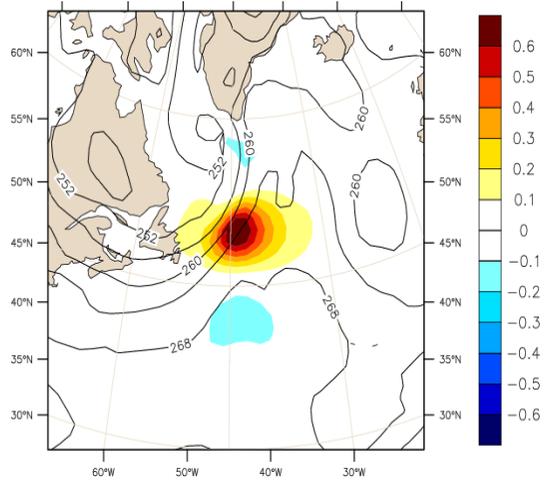
- Evolutionary (not revolutionary) path from VarDA to EnDA for operational NWP as future computers allow larger ensembles.



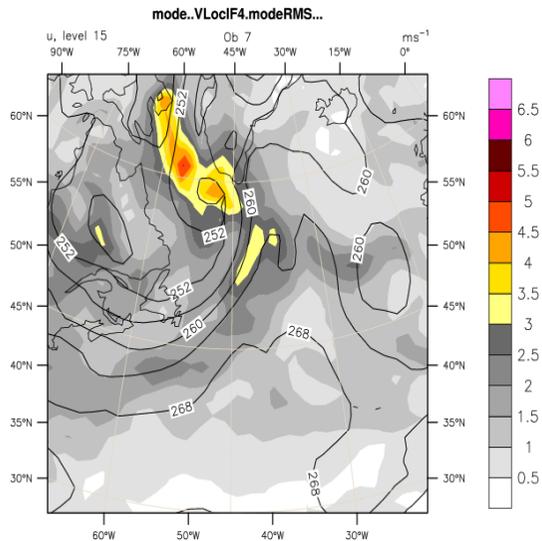
# Single Observation Tests: $\langle u u \rangle_h$



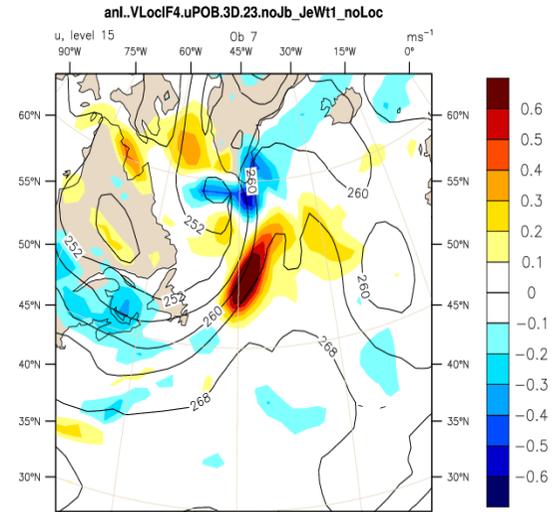
3D-Var Increment



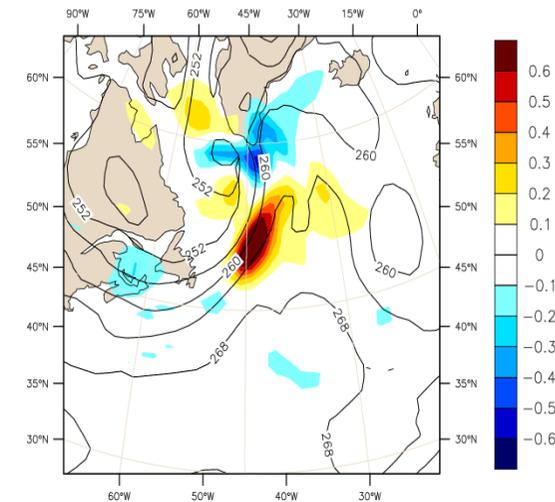
© Croi 4D-Var Increment (middle of 6hr time window)



Ensemble Spread



Ensemble Increment,  $A=I$



Ensemble Increment,  $A=A_h$

Adam Clayton

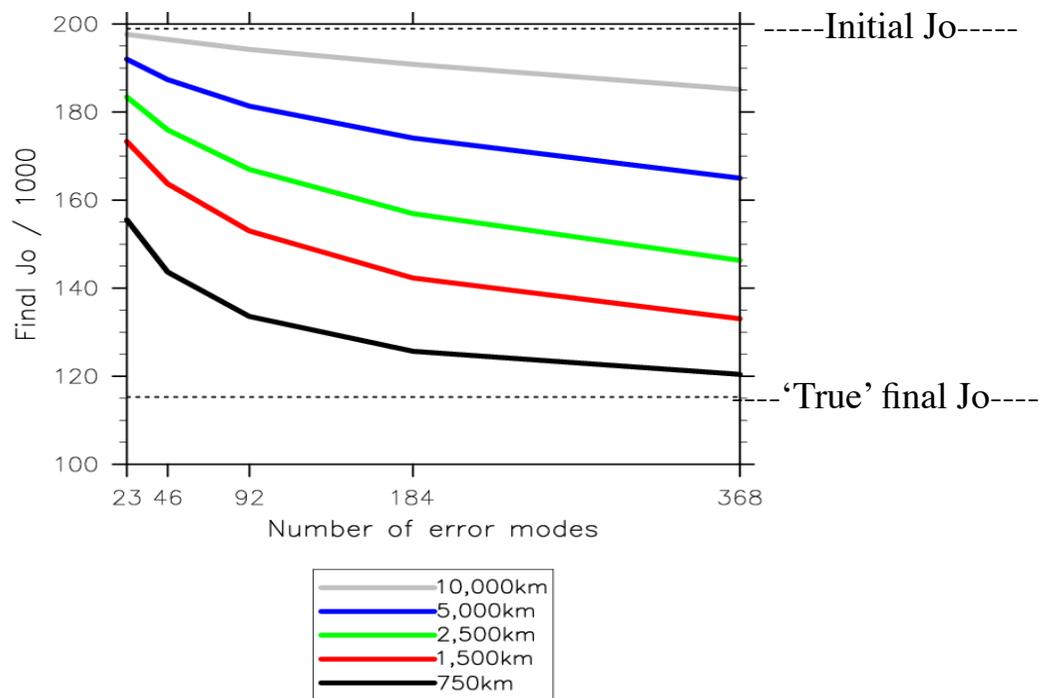


Met Office

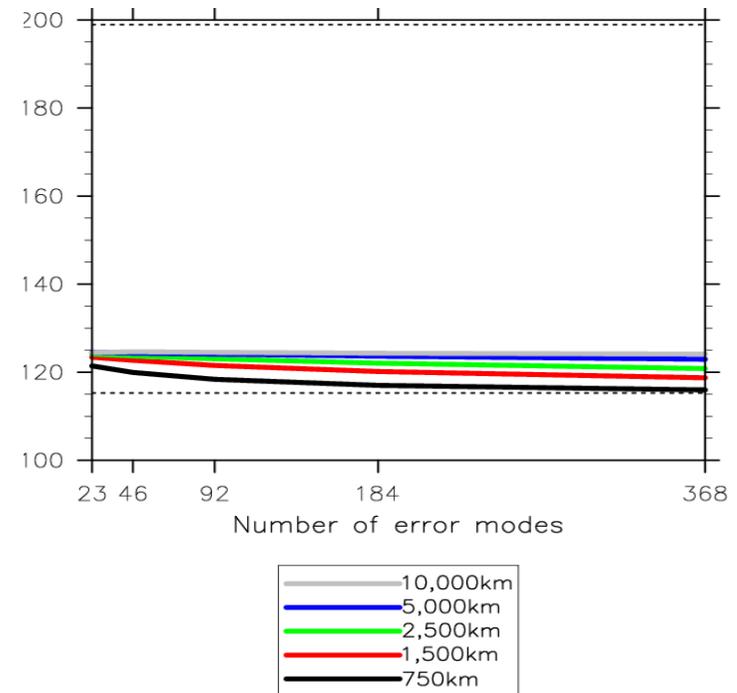
# Estimation of Ensemble Sampling Error

**Method:** Simulate ensemble by sampling climatological **B**. Study effect of ensemble size, localization, hybrid on minimization.

Pure Ensemble Covariance



Hybrid Covariance



- Pure ensemble covariance still significantly underfitting observations, even with  $O(400)$  ensemble members, and reduced localization scales.
- **Hybrid approach likely to be valid for the significant future.**



# EnDA: The contenders

Good, Bad (only sample of issues shown)

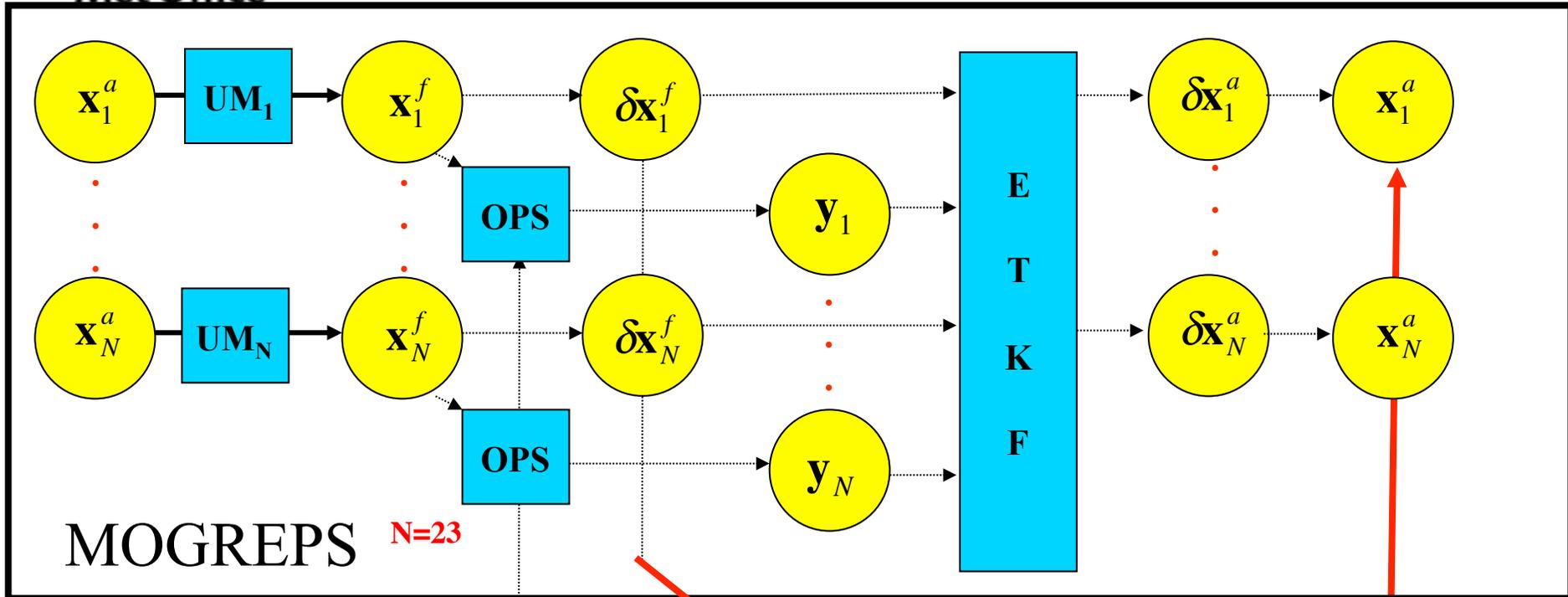
- Hybrid 3/4D-Var + EnsFilter (MetO + NCEP, NRL, HIRLAM, etc)
  - Reaps benefits of variational framework (e.g. outer-loop, Huber norms, etc).
  - Hybrid forecast error covariances ameliorate ensemble sampling error.
  - Model-error treatment possible through weak-constraint formulism.
  - Inconsistent Kalman Gain between DA and EPS - two DA algorithms.
  - Computational efficiency compromised by 4D-Var scalability and scheduling.
  - Inflexible to alternative model/application.
  - ETKF Localization issues (could replace with e.g. EnSRF).



# MetO: EnDA = Hybrid 4D-Var/ETKF

$$\mathbf{y}_n = H(\mathbf{x}_n^f), \sigma_o, \dots$$

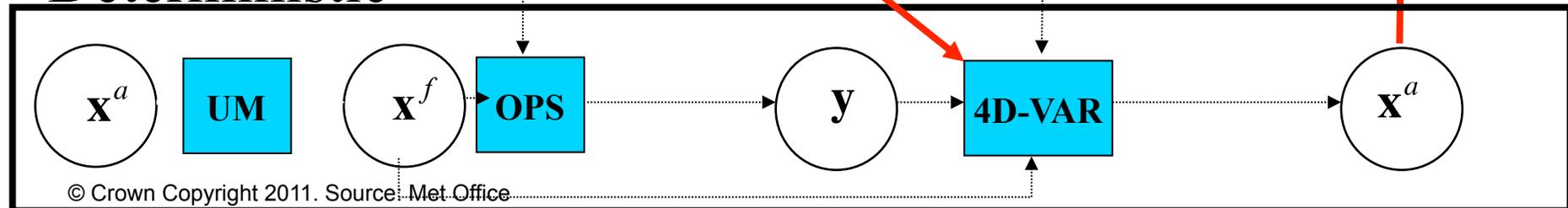
$$\mathbf{x}_n^a = \mathbf{x}^a + \delta\mathbf{x}_n^a$$



(UM = Unified Model)

(OPS = Observation Preprocessing System)

## Deterministic





# EnDA: The contenders

## Good, Mixed, Bad

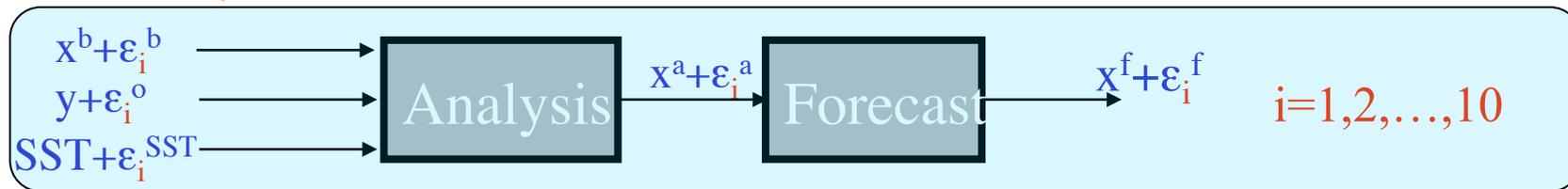
(only sample of issues shown)

- EnKF - Serial EnSRF, Serial EnKF, ETKF, EAKF, LETKF, MLEF, EnKF-GLS
  - Bypasses need to develop adjoint/linear model (but still need covariance modelling).
  - Scalable (at least forecast step), flexible.
  - Consistent Kalman Gain between DA and EPS.
  - Increased reliance on input data (ensembles) rather than explicit DA modelling.
  - Does not reap benefits of variational framework (e.g. simultaneous treatment of obs).
  - Model-error and sampling error confused during inflation process.
  - Can reproduce/improve EnKF with hybrid, so why bother?

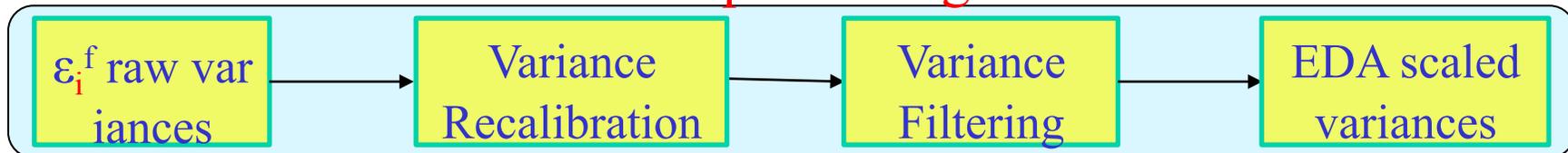


# MF/ECMWF: EnDA = Ensembles of 4D-Var (Courtesy Lars Isaksen)

EDA Cycle: 10 x Low-Res T95/159 4D-Var. Perturbed obs/SSTs:



Forecast Error Variance Post-processing:



High-Resolution Deterministic 4D-Var Cycle:





# EnDA: The contenders

Good, Bad (only sample of issues shown)

- Ensemble of Weak-Constraint 4D-Vars (e.g. MF, ECMWF)
- Reaps benefits of variational framework.
- Model-error treatment possible through weak-constraint formulation.
- DA scalable (small ensemble+WK4DV).
- Consistent Kalman Gain between DA and EPS
- Analysis step costly compared to forecast step.
- Inflexible to alternative model/application (OOPS will help).
- Limited ensemble size (e.g. 10) enables only conservative use of ensemble covariances (e.g. variances, lengthscales, etc).



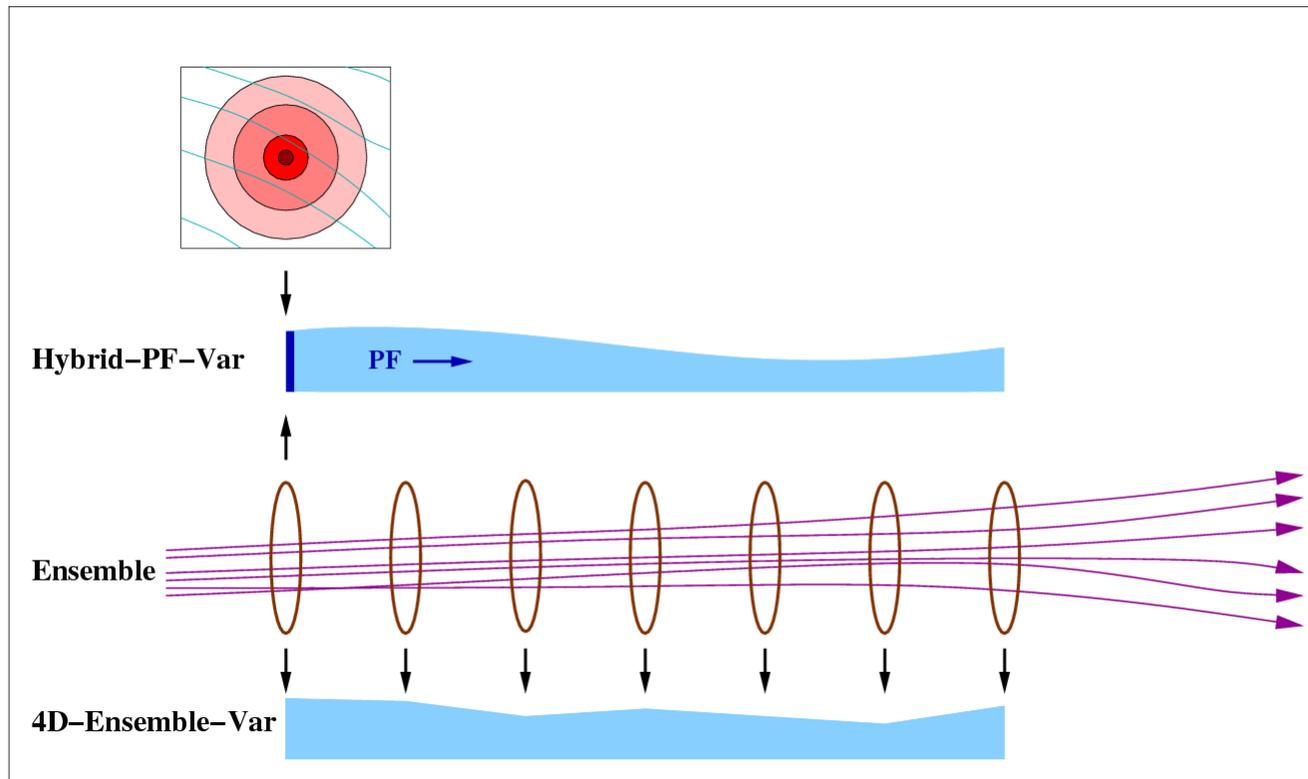
# EnDA: The contenders

Good, Bad (only sample of issues shown)

- Particle filter
- True nonlinear/non-Gaussian DA.
- DA scalable, flexible.
- Pure PF unaffordable (the ‘curse of dimensionality’ – will never be able to afford pure PF for NWP).
- Does not reap benefits of variational framework. Radical, risky change at present!
- Perception that PFs are still a black art? ‘You can do what you like’ – Peter Jan.
- Promising results combining PF ideas with e.g. nudging, WEnKF, 4D-Var (but practical solutions may not be that different to other current options e.g. ensembles of 4D-Var, hybrid nudging-EnKF systems, etc).

# EnDA: The contenders

- Ensemble of 4D-Ensemble-Var (Var mimicking the EnKF):





# Comparison of Hybrid 3/4D-Var and 4D-Ensemble-Var (Buehner et al 2010)

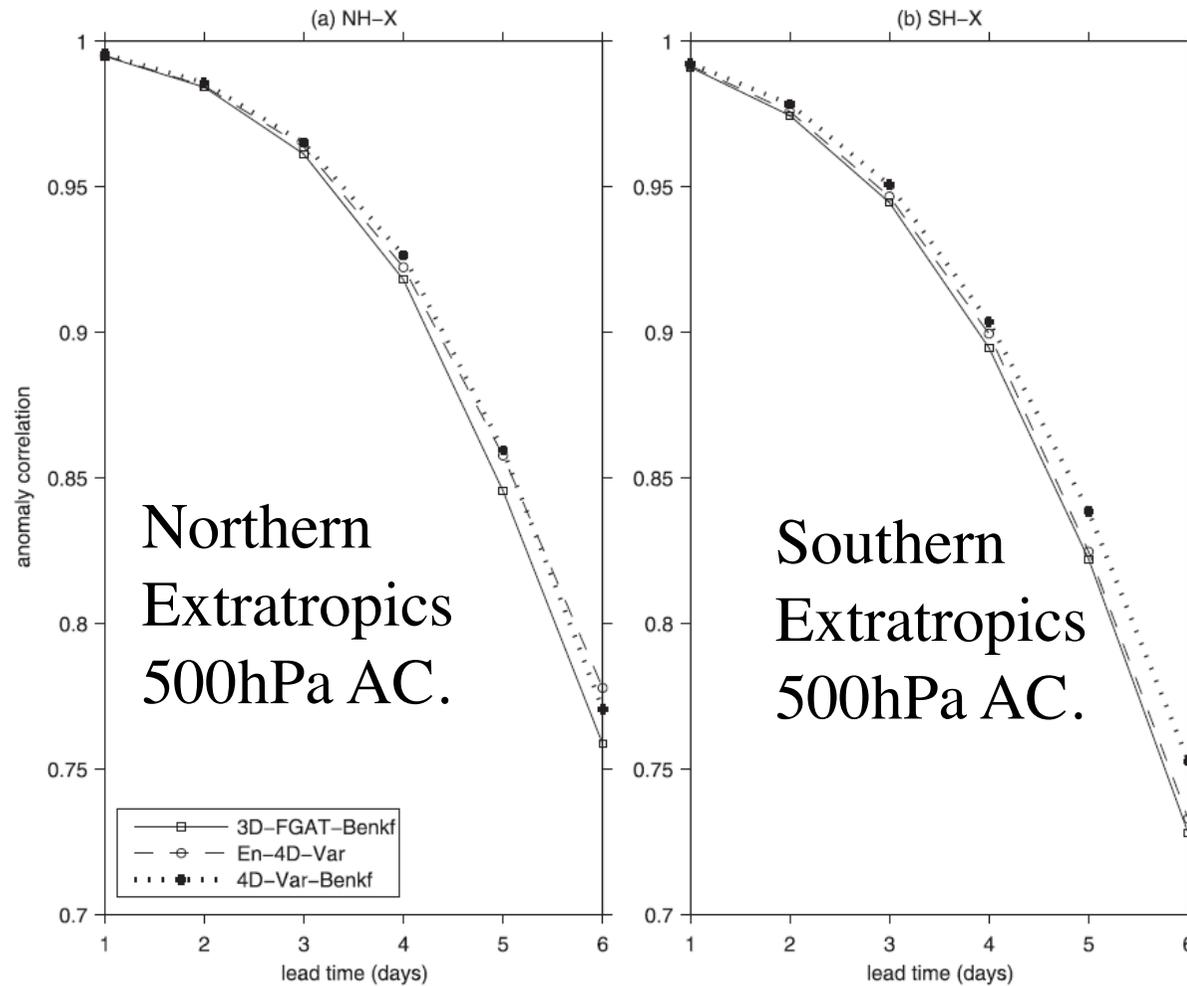


FIG. 12. As in Fig. 6, but for the 3D-FGAT-Benkf (solid), En-4D-Var (dashed), and 4D-Var-Benkf (dotted)

4D-Ensemble-Var (dashed), Hybrid 4D-Var (dotted), Hybrid 3D-Var (solid).



# EnDA: The contenders

Good, Bad (only sample of issues shown)

- 4D-Ensemble-Var (Var mimicking the EnKF).
  - Reaps benefits of variational framework (including e.g. outer-loop).
  - Bypasses need to develop adjoint/linear model.
  - Model-error possible through weak-constraint formulism (e.g. MECV).
  - DA scalable, flexible.
  - Hybrid forecast error covariances (natural extension to current hybrid).
  - Minimization cost similar to 3D-Var, EnKF – significantly less than 4D-Var.
  - Increased reliance on data (ensembles) rather than physical knowledge (linear model, balance) to provide covariance info.
  - Large I/O and memory requirement.
  - Output is not a model solution. Where to start forecast?
  - Inconsistent Kalman Gain between DA and EPS (solution: ‘Ensemble of 4D-Ensemble-Vars’).



# Strategy Going Forward

- Improve 4D-Var efficiency: SE + algorithmic changes + leave door open for potential ensemble of WK4DV as 'plan B'.

## Plan A:

- Continue to develop hybrid for short/medium-term (1997-2015):
  - Increase ensemble size, more sophisticated localization, etc.
  - Consider replacing ETKF as ensemble perturbation generator.
  - Develop convective-scale hybrid 3/4D-Var (2012-2015).
- Develop 4D-Ensemble-Var for medium/long-term:
  - Code and test within current VAR framework (2011-2012).
  - Extend to an 'Ensemble of 4D-Ensemble-Vars' (2012-2015).
  - Retire PF model if/when 4D-Ensemble-Var beats 4D-Var.



# Summary

- DA continues to provide major NWP performance improvements.
- 4D-Var/EnKF competitive. Combination even better.
- Practical issues (cost, maintenance, flexibility, scheduling) have major impact on strategy for operational NWP.
- Many centres opting for 'Ensemble Variational Data Assimilation' as way forward.
- For MetO, plan A is hybrid, then 4D-Ensemble-Var if beats hybrid 4D-Var.